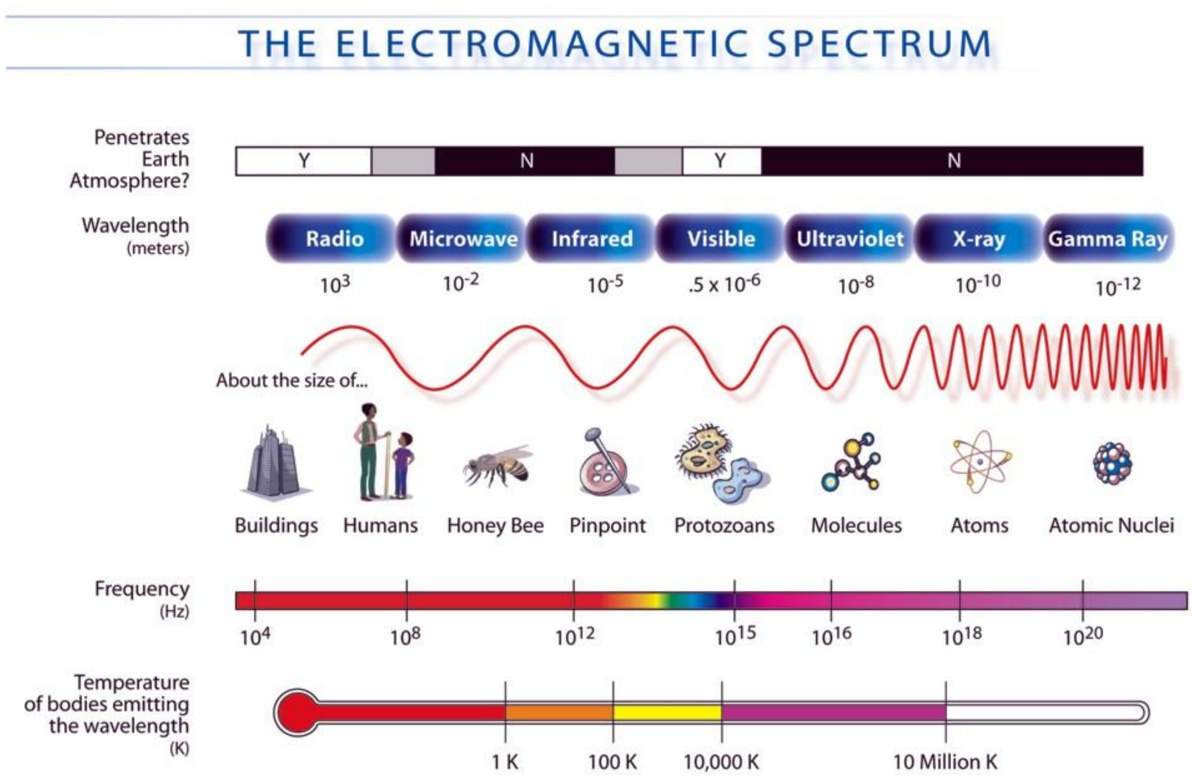
1. Spectroscopy – frequency dependence of the interaction of light with matter
   1.1. Absorption (excitation), emission, diffraction, scattering, refraction
   1.2. Interaction with molecular species
      1.2.1. wavelength depends on (molecular) energy levels that are available
      1.2.2. Depends on structure
2. Available frequencies and corresponding molecular absorption processes
   2.1. Radio waves - nuclear spin states
   2.2. Microwave – rotation and electron spin states
   2.3. Infrared – vibration states
   2.4. Optical (visible and ultraviolet) – valence electronic states
   2.5. X-ray – atomic core electronic states
   2.6. Gamma – nuclear states



http://mynasadata.larc.nasa.gov/images/EM_Spectrum3-new.jpg

3. properties of light

3.1. $E = h\nu$, $\nu = c/\lambda$, $E = hc/\lambda$

3.1.1. $E = \frac{28600(nm \cdot kcal/mol)}{\lambda(nm)}$

3.1.2. 300 nm = 95.3 kcal/mol

3.1.3. 600 nm = 47.7 kcal/mol

3.1.4. 2000 cm^{-1} = 5 μ = 5.7 kcal/mol

3.1.5. 500 MHz = 4.8 x 10^{-5} kcal/mol

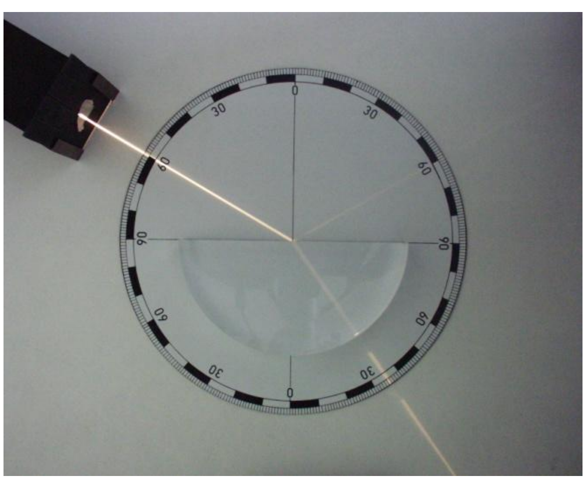
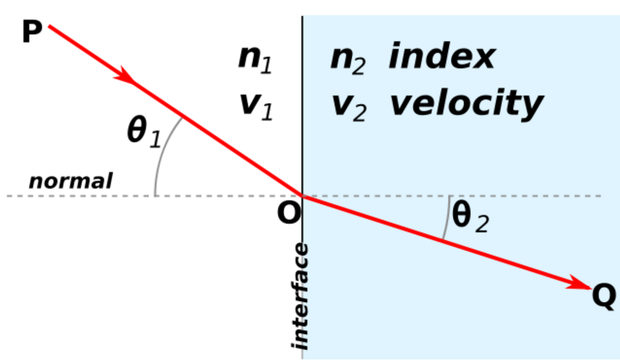
3.2. $E = h\nu$ indicates light has wave-like properties

3.2.1. Frequency: $\nu = E/h$

3.2.2. $\lambda\nu = c$, $\lambda = c/\nu$ = wavelength, $\lambda = hc/E$

3.3. Refraction – bending of light upon passing between two mediums of different refractive indexes

3.3.1. Snells Law: $\frac{sin\theta_1}{sin\theta_2} = \frac{n_2}{n_1} = \frac{v_1}{v_2}$ of http://en.wikipedia.org/wiki/Refraction, http://interactagram.com/physics/optics/refraction

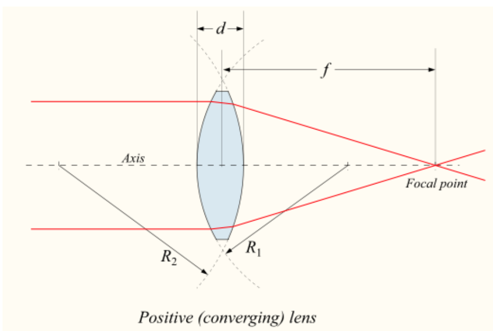
3.3.2. Bending of light depends on medium and frequency

3.3.3. Prism – bends light depending on wavelength,

http://en.wikipedia.org/wiki/File:Light_dispersion_of_a_mercury-vapor_lamp_with_a_flint_glass_prism_IPNr%C2%B00125.jpg

3.3.4. Lens – curved surface, collects parallel light beams – focus,

http://en.wikipedia.org/wiki/File:Lens1.svg



3.3.5. Accompanied by reflection

3.4. Reflection - angle of incidence = angle of reflection

3.4.1. frequency unchanged for incident and reflected photons

3.4.2. Amount of reflection and refraction depends on angle wavelength and difference in refractive index

3.4.3. Reflection increases with decrease incidence angle and difference in refractive index

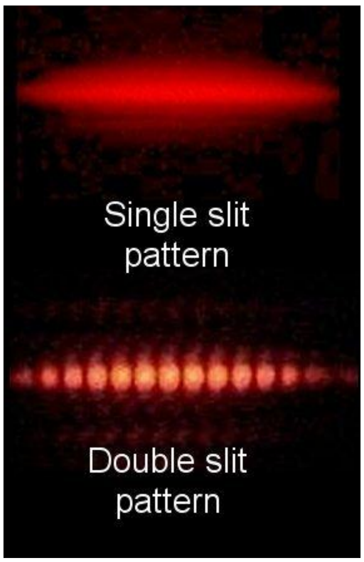
3.4.4. What happens when refractive indexes are the same?

3.4.5. Metallic coating suppresses wave propagation

3.5. Diffraction – bending of light as it passes around the edge of an object

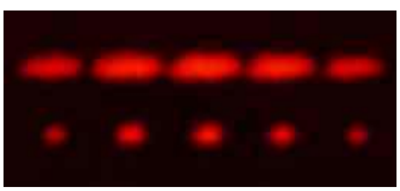
3.5.1. The amount of bending depends on the relative size of the wavelength of light to the size of the aperture. Image broadens as aperture size approaches wavelength size.

3.5.2. http://en.wikipedia.org/wiki/File:Doubleslit.gif, http://en.wikipedia.org/wiki/Diffraction

3.5.3. 

What causes alternating intensity?

http://en.wikipedia.org/wiki/File:Single_and_double_slit_4.jpg


double versus 5 slits: better resolution

http://en.wikipedia.org/wiki/Diffraction#mediaviewer/File:Diffraction2vs5.jpg

3.5.4. Relevant parameters?

3.5.5. $d(\sin\theta_m + \sin\theta_i) = m\lambda$, d = slit width, θ_i = angle of incident light relative to surface; θ_m = angle of diffracted light, m = order (integer), for θ_i = 90, then $\sin\theta_m = \frac{m\lambda}{d}$

3.5.6. Multiple slits improves separation of multiple wavelengths

3.5.7. Absorption – light converted to potential energy or heat

3.5.7.1. Change of temperature – translational- mostly

3.5.7.2. Change of state – electronic, vibration, rotation

3.6. Photon energy is quantized therefore absorption process must be quantized

3.7. oscillating magnetic and electric fields

3.7.1. perpendicular to each other

3.7.2. perpendicular to the direction of propagation

3.7.3. electric dipole

3.7.4. angular momentum

4. When is light absorbed?

4.1. Answer Q: what happens when light is absorbed?

4.2. Molecule moves from one quantum state to another

4.3. Molecules only have discrete energy states

4.3.1. electronic, nuclear, vibrational, rotational, translational

4.4. .difference in energy states must equal photon energy

5. States of molecules

5.1. Sum of rotation vibration, electronic, ignore translation and nuclear for now

$E_{tot} = E_{rot} + E_{vib} + E_{el}$

5.2. Energy changes can occur by absorption or emission of photon

5.3. $h\nu = (E^1_{rot} - E^2_{rot}) + (E^1_{vib} - E^2_{vib}) + (E^1_{el} - E^2_{el})$

5.4. interpretation less specific at higher energies

6. particle in a box

6.1. approximate an atom – electron confined in a small space

6.2. particle confined along a distance a

6.3. potential energy U = 0 for position x = 0 to a, infinite everywhere else

6.4. probability of particle being in the box is 1

6.5. determine wave function ψ for a particle – spatial distribution- use Schrodinger wave equation

6.6. $\frac{d^2\psi}{dx^2} = -\frac{8\pi^2 m}{h^2} E\psi$ m = mass, h = Planck's constant, E = energy

6.7. Solution is $\psi = A \sin\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} x + A' \cos\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} x$

6.8. Wave function must be 0 for x = 0 therefore A' must be 0

6.9. Wave function must be 0 for x = a,

$\sin\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} a = 0$,

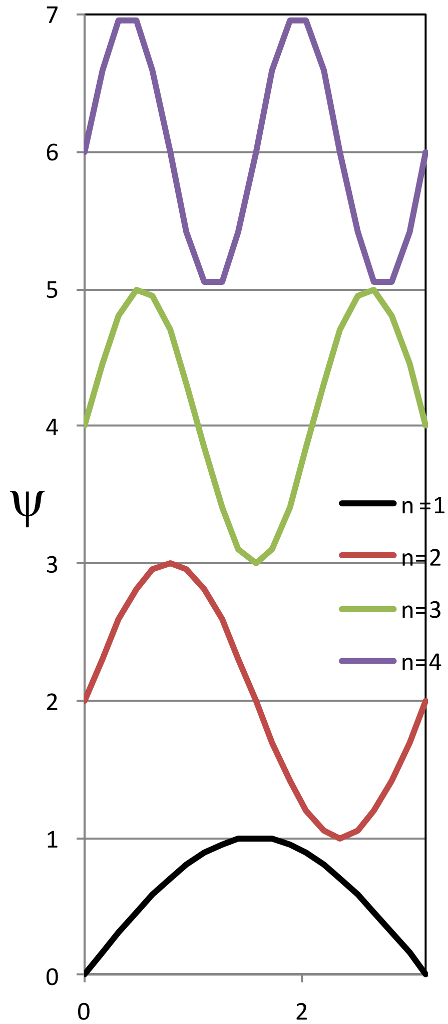
if $\left(\frac{8\pi^2 mE}{h^2}\right)^{1/2} a = n\pi$ square both side then …

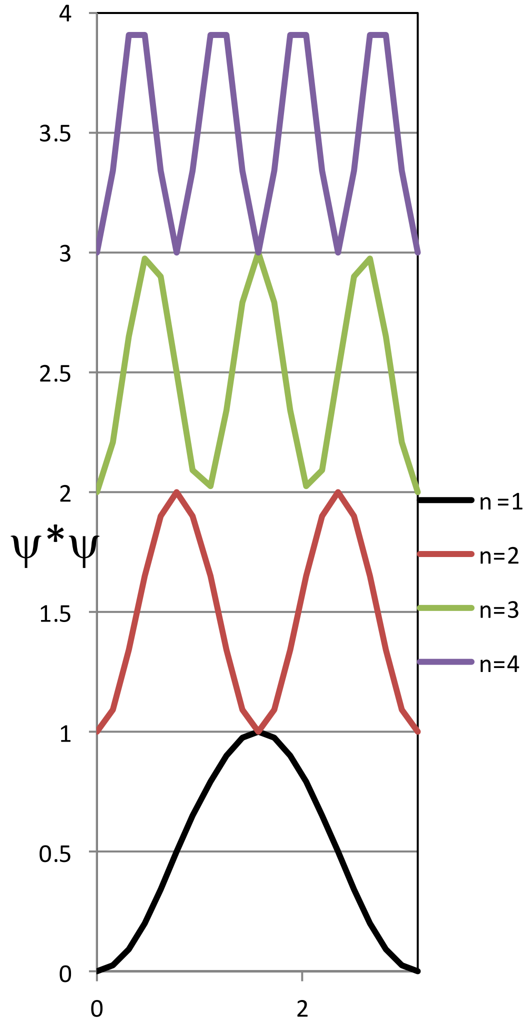
6.10. $E = \frac{h^2 n^2}{8ma^2}$, particle can only have energies for integer values of n

6.11. Energy increases with n^2: 1, 4, 9, 16, 25, 36, 49, 64, etc.

6.12. Wavelength = 2a/n

6.13. Bigger the box or heavier the particle the more closely space energies





6.14. Number of nodes increases with n.

6.15. Common trend no matter what the boundary conditions or how "box" is constructed, for example, overlapping several p orbitals (π bonds)